The 12th international conference Distillation & Absorption 2022
Toulouse – France 18-21 September 2022

Vapor Recompression: An interesting option for vacuum columns?

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Abstract. The need to reduce greenhouse gas emissions and the use of fossil fuels will greatly change the design of process plants. Besides improved heat-integration, an obvious option to this goal is the use highly efficient and therefore smart electrification. Hence, heat pumps and vapor recompression systems effectively recirculating energy flows may become economical in applications where experience had quickly eliminated them in the past. In this changing socio-economic context, process engineers will have to re-think, challenge and even un-learn many accepted design practices. One example is the use of vapor recompression in distillation. While applications in close-boiling pressure systems have been reported in literature, the number of actual realizations is comparatively small. In vacuum systems, the practical hurdles are even higher, since the large volumetric flowrates result in high compressor investment. In this paper, alternative designs opening the way to electrification for a well-known vacuum system are presented.

Keywords: vapor recompression, distillation, heat pump, heat integration, electrification, working fluid

Introduction

The energy saving potentials of heat pump systems in distillation have been known for more than half a century (1). Three basic schemes, direct vapor recompression (VR), bottom flashing and heat pumps (HP) using a suitable working fluid have been proposed by Null (2). In all cases, mechanical energy is used to increase the condensation temperature of a vapor stream so far, that it can be utilized to heat the reboiler. In some cases, thermal vapor recompression with ejectors may be a capital saving alternative to turbo or piston compressors (3). Since the difference between the boiling points of bottom and top directly influences the required compressor power, most published cases have focused on close-boiling mixtures. Superfractionators like C3-splitters are predominant in literature studies. High reflux ratio and vapor density make them obvious candidates for vapor recompression or heat pumps (4, 5). In a recent review (6), different heat pump assisted configurations including absorption heat pumps and internally heat-integrated columns (HIDIC) are examined. In a comparative optimization study, Harwardt and Marquardt (7) conclude, that VR and HIDIC are more economical than conventional columns only for close boiling mixtures, VR being more cost-efficient than HIDIC. Two examples for atmospheric and vacuum systems with pay out times of about two years are given by Ferré et al. (8).

While direct heat-integration is well established in industry (9), only few industrial columns are equipped with heat pumps despite the unanimously encouraging literature results. Many practical concerns are hindering its widespread exploitation. Compressors are expensive, long-lead items. Detailed supplier know-how on compressor cost and performance curves, which is required to find optimum overall designs, is not freely available. Furthermore, application to thermally sensitive, corrosive, or polymerizing systems is challenging. In vacuum systems, low vapor density leads to high volumetric flowrates to be compressed and high compression ratios resulting in high investment for the compressor and associated large-diameter piping. These reservations often lead to premature exclusion of VR or HP options in early project stages.

In this paper, an ethylbenzene / styrene monomer column is investigated as an example to explore the energy- and CO_2-saving options accessible by VR and HP configurations in vacuum systems. One option is to increase column top pressure to the highest allowable value from polymerization considerations in a VR configuration. An alternative is the use of a closed-cycle heat pump for which several possible working fluids are examined.

Detailed simulations comparing a conventional vacuum column, VR and HP systems at deep vacuum as well as elevated pressures are performed. Relative merits and drawbacks of the column configurations are investigated, and a basic economic analysis is presented. It is shown, that even in vacuum systems, carefully designed VR or HP systems open large potentials to reduce CO_2 footprint and offer an important key technology on the way to a smart and sustainable electrification of the process industries.

Example Process

Depending on the desired product purity, distillation of ethylbenzene (EB) and styrene monomer (SM) requires about 70 to 90 theoretical stages. Historically, low pressure drop sieve trays at low flooding factor were employed. The allowable top pressure was restricted to about 80 mbar to keep the bottoms temperature below 110°C to limit polymerization of styrene utilizing suitable stabilizers (10). The dehydrogenation reaction yields feed concentrations of about 43 w-% EB, 55 w-% SM and 2 w-% others. Meanwhile, the advent of structured packing of low pressure drop allowed capacity increases and lower bottoms temperature at the same time (11, 12), enabling some licensors to offer heat-integrated double-effect column systems saving energy, CO_2 emissions and cost (13).

In this paper, a column separating a saturated binary feed stream of 50,000 kg/h containing 45 w-% EB into a distillate of 99.5 w-% EB and a bottoms product of 99.8 w-% SM purity is investigated. Vapor recompression and heat pump systems at various column pressures are compared using ASPEN plus Radfrac models with the property method SRK. Diameters and pressure drops are estimated for ≈72 % flooding factor for 250 m^2/m^3 high capacity structured packing using ASPEN hydraulics validated with Sulcol (14). Compressors are modelled isentropic with the ASME method specifying isentropic and mechanical efficiencies of 85 and 95 %, respectively.

In a conventional, simple column configuration, it is straightforward to select the lowest operating pressure allowing for cheap condensation using an air cooler. At about 80 mbar, a low bottom temperature results, limiting by-product formation and increasing the chance to re-use waste heat streams of suitable temperature. While all these arguments are in favor of low vacuum operation, there is room to optimize the column pressure under new energy supply and cost conditions at least up to the bottom temperature witnessed in the trayed designs used in the past. For a C3-splitter, Muhrer (15) demonstrates how vapor recompression may make a wider range of column pressures accessible for economic optimization.

Important column design parameters are given in **Table 1** for three pressures. As pressure is increased, relative volatility decreases, requiring a higher number of theoretical stages. Reflux ratio and reboiler duty both increase, while tower diameter can be decreased. At 300 mbar, the bottoms temperature exceeds the limit of 110°C, while a considerable margin remains at 220 mbar (e. g. for pressure drop higher than estimated).

Table 1.
Column design parameters

Pressure [mbar]	Rel. volatility [-]	# theor. stages [-]	Top temperature [°C]	Bottom temperature [°C]	Reflux ratio [-]	Reboiler duty [MW]	Diameter [mm]	Compression ratio [-]
80	1.4	70	62.4	82.9	6.75	18.5	5,800	3.32
220	1.35	80	87.8	103.7	7.43	19.5	5,050	2.38
300	1.33	84	96.6	110.7	7.66	19.7	4,900	2.16

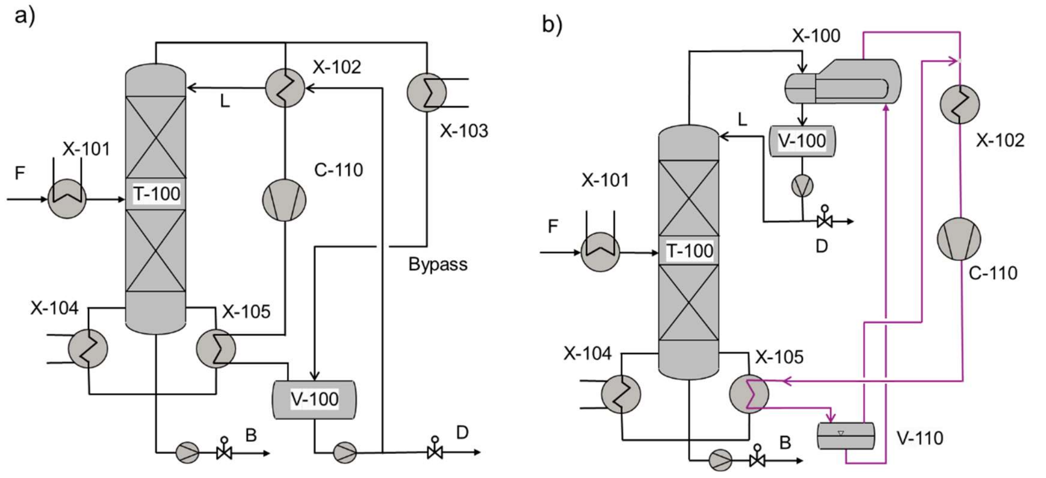

Fig. 1: Flowsheet of a) vapor recompression and b) heat pump configurations. Working fluid piping shown in purple.

Fig. 1 shows flowsheets for VR and HP configurations. In both configurations, the feed is preheated to the boiling point in X-101 and a start-up reboiler X-104 is shown. In **Fig 1 a)**, the overhead vapor is superheated in X-102 and compressed in C-110 so far, that a driving temperature difference of 10 K is available in X-105 (reboiler). In X-102, the overhead vapor is superheated to avoid condensation during compression.

Although the reflux is cooled in X-102 and in X-101 (not shown in Fig. 1 for clarity), it is still superheated at column top conditions and partially flashes. To limit the additional flow to the compressor to the rate required to heat the reboiler, a trim cooler X-103 is installed to remove excess duty from the system. In **Fig. 1 b)**, a heat pump configuration is shown. Here, the overhead stream is condensed inside the tubes of a kettle exchanger X-100 while the heat pump's working fluid is evaporated on the shell side. Again, the working fluid is compressed in C-110 and used to heat reboiler X-105. The condensate is flashed into V-110. A part of the residual vapor stream is recycled to X-102 to provide enough heating duty in X-105. The trim condenser is not shown here.

Vapor recompression (VR) and heat pump (HP) systems

Simulation results for the VR configuration for six selected column pressures from 80 to 300 mbar are shown in **Fig. 2**. Since column designs (# of stages, reflux ratio, diameter etc.) have been adapted individually for all pressures, the results are shown as symbols interpolated by lines. As pressure is increased, compressor duty and compression ratio decline significantly. The coefficient of performance (COP, the ratio of units of reboiler duty recycled to mechanical power supplied to the compressor) rises from about 8 to almost 12 (see **Fig. 2a**). The reason is clearly visible in **Fig. 2b**: While the mass flowrate to be compressed increases with pressure by about 10% (due to higher reflux ratio), the volumetric flowrate declines considerably to less than a third. Both effects decline above ~200 mbar.

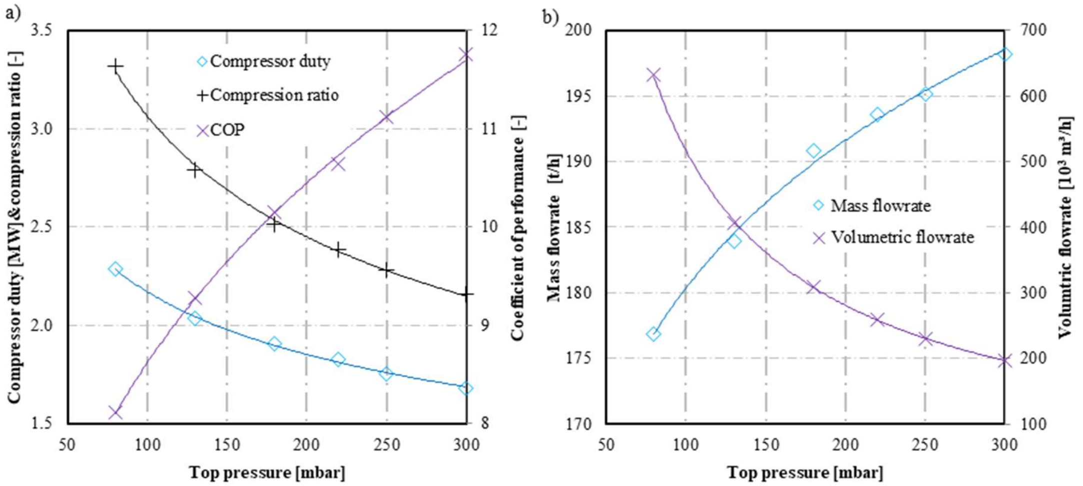

Fig. 2: Influence of column pressure on main VR design: a) COP rises with column pressure while compression ratio and compressor duty decline; b) although overhead vapor mass flowrate increases with pressure, volumetric flowrate declines.

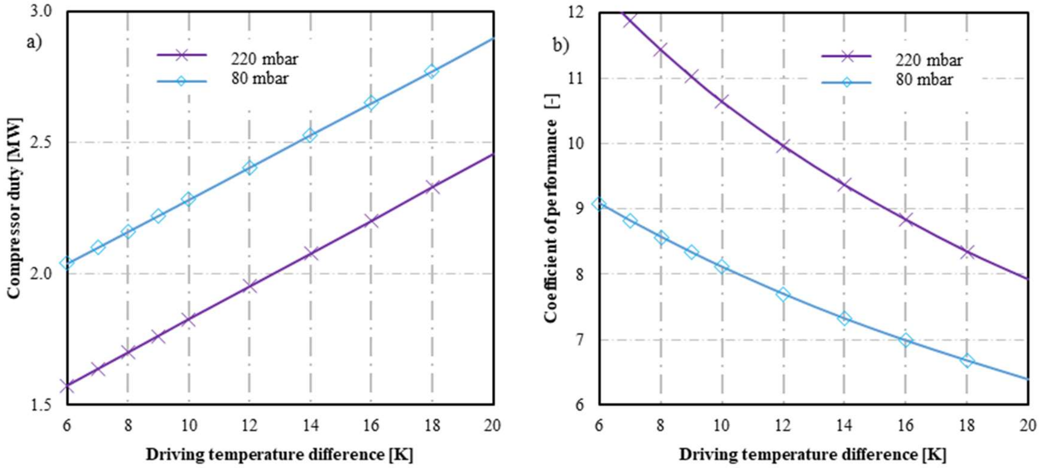

Fig. 3: Impact of driving temperature difference in reboiler X-105 on a) compressor duty and b) COP

The effect of the driving temperature difference in reboiler/condenser X-105 is shown in **Fig. 3** for two selected column pressures of 80 and 220 mbar (the effect of the superheated nature of the vapor from compressor C-110 is neglected). For both pressures similar trends are observed. Compressor duty rises with temperature difference while COP declines. The clear advantage for the higher pressure column is due to the fact, that the temperature difference between bottom and top is more than 5 K lower than in the lower pressure case, resulting in a lower compression ratio (**Table 1**).

If the overhead product is sensitive to polymerization or thermal degradation, a closed-cycle heat pump system may be beneficial. The choice of an optimal working fluid is decisive. Three classes of working fluids are considered here. Hydrocarbons are often denoted as natural working fluids, have low global warming potential (GWP) and ozone depletion potential (ODP) and are common substances in chemical plants. The alkanes propane to n-heptane are investigated. Chlorofluorocarbons (CFC) like R21 have proven their efficiency as classical refrigerants but are now prohibited or facing phase-out due to their high GWP. Hydrochloroflouroolefins like R1233zd(E) and R1234ze(E) share many of the positive thermodynamic properties of CFCs. Moreover, the double bond in these molecules makes them easily degradable in the atmosphere and make them promising substitutes for CFCs (16). All these working fluids have hanging *log(p),h*-diagrams. The more this feature is developed, the higher is the degree of suction side superheating required to avoid condensation during compression (16). Methanol, on the other hand, has a bell-shaped *log(p),h*-diagram requiring no superheating at all. Since only very small pressure drops may be allowed in vacuum systems, large superheating requirements lead to large superheater areas.

A comparison of COP values is given in **Fig. 4 a)**. Generally, COP is larger for the higher pressure case. Since two driving temperature differences must be overcome in X-101 and X-105, respectively, the VR configuration outperforms the HP configurations in all cases. Propane and R1234ze(E) have a low critical temperature and are unfavorable even in the 80 mbar case, while no sub-critical condensation is possible in the 220 mbar case. Results for the other working fluids are quite similar. COP increases with chain length for the hydrocarbons. While no advantage is visible for the fluorinated compounds, methanol gives the highest COP of all working fluids. A comparison of COP alone, however, does not give the full picture, as **Fig 4 b)** shows. The volumetric heating capacity is the ratio of reboiler duty to compressor suction volume flowrate (16). The higher this value, the smaller the size of compressor and associated piping and exchangers. While the higher pressure cases still give higher values, the ranking of working fluids is completely different. VR and the long chain hydrocarbons show the smallest values, since the suction side vapor densities are quite small. For butane and refrigerants like R21 or R1234zd(E), the highest values result. Obviously, an economic analysis is required to identify optimum solutions.

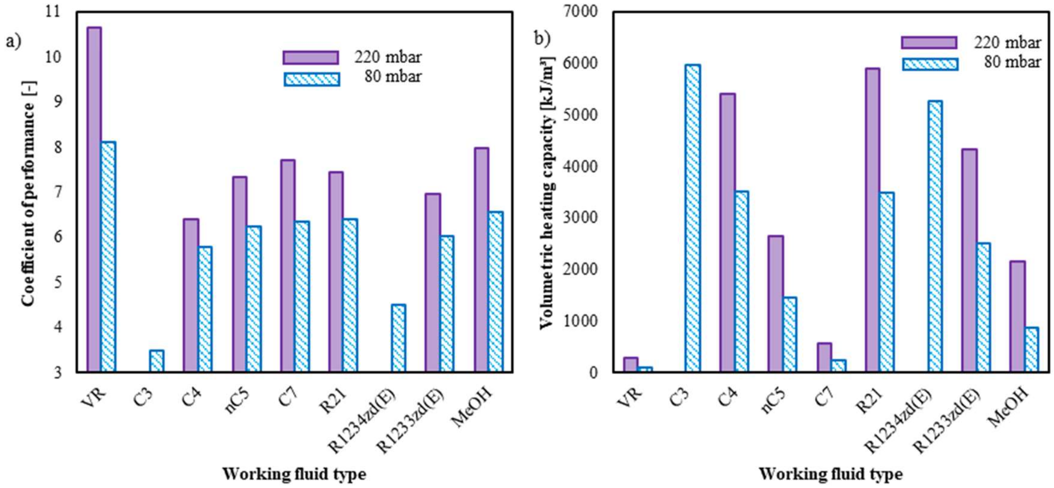

Fig. 4: Impact of working fluid on a) COP and b) volumetric heating capacity of HP and VR configurations.

Economic analysis

VR and HP configurations require considerable additional investment compared to a simple column system. To quickly assess the economics of all cases presented, cost functions for columns and heat exchangers given by Luyben (17) are slightly adapted and supplemented by own estimates of packing cost. In literature correlations, the only variable determining compressor cost is its duty. As pointed out by Luyben (18), this is a serious shortcoming, since suction pressure (i.e. suction gas density) has a significant influence on compressor size. This conclusion is consistent with Evonik project experience. Therefore, a cost function correlating both power and suction side density was fitted to our limited in-house data on large turbo compressors cost.

For the simple column, a large, air-cooled condenser is required, which is replaced by the much smaller trim condenser in the VR and HP cases. However, due to lower driving temperature difference, the reboiler X-105 is several times larger in VR and HP configurations. In HP systems, this large exchanger is required twice, X-100 for evaporation and X-105 for condensation of the working fluid. The largest investment cost differences are caused by the compressor itself, its electric power supply, as well as additional heat exchangers and large diameter piping. Based on simulation data, equipment sizes were determined and used to estimate equipment cost. A factor of 3.3 is used to estimate total plant cost. Cost of the working fluid was neglected.

With energy prices of 50 €/MWh for electric energy and 25 €/MWh for steam, Pay Out Time (POT) was computed by dividing the additional total plant cost of VR and HP configurations compared to the simple column by the amount of energy cost savings. To estimate a Net Present Value (NPV), an internal interest rate of 15% and a plant run time of 10 years was assumed.

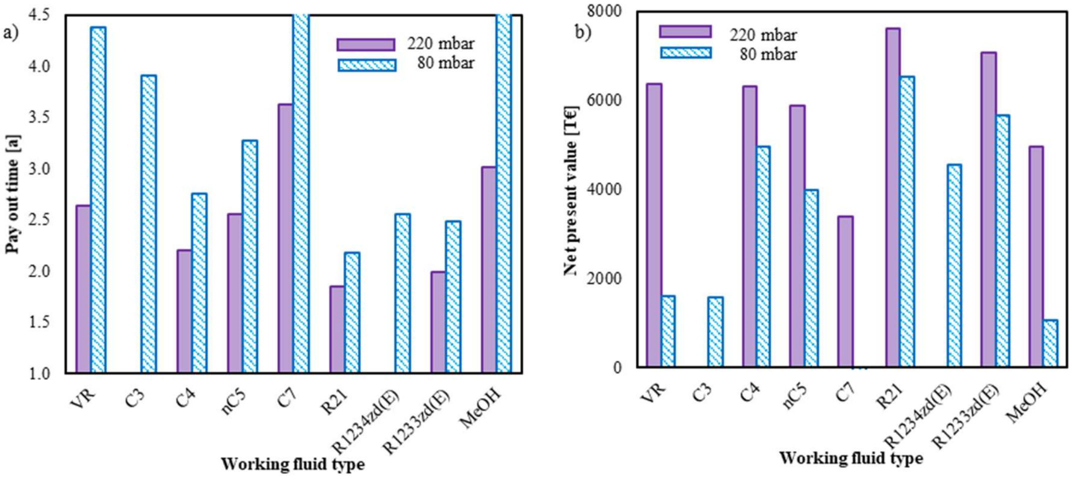

Fig. 5: Pay out time and net present value for VR and HP configurations for two column pressures.

Results for POT are shown in **Fig. 5 a)**, while **Fig. 5 b)** gives the NPV. Keeping in mind, that the full energy saving potential at 100% plant capacity was exploited in the analysis, it is clear, that both POT and NPV values shown must be considered as optimistic. However, some important conclusions may be drawn:

- Use of HP and VR configurations can save 75 to 85% of CO_2 emissions. Using green electricity, CO_2 emission-free separation is possible.
- The economic ranking in Fig. 5 consolidates the conflicting rankings found in Fig. 4 a) and b). A purely thermodynamic analysis is insufficient, high COP values do not guarantee economic designs.
- The higher pressure designs show considerably better economic feasibility.
- This clearly shows that simply imposing VR or HP options on an optimized simple column design will not necessarily lead to an optimum design. To fully exploit the savings potential, the complete range of allowable operating conditions needs to be evaluated.
- HP configurations show better economics than VR in the 80 mbar case. At the higher pressure, VR gains ground.
- The high pay out time for the lower pressure VR configuration may explain, why there are very few vacuum VR columns in operation.
- With rising CO_2 cost and trend to electrification, this assessment can be expected to change.
- While the COP of the working fluids showed little difference, the traditional CFC refrigerants show better economics. This is largely due to higher volumetric heating capacity and consequently lower compressor investment.
- The compressor is the dominating element of the additional VR or HP investment costs. Results from available literature cost models significantly disagree, causing uncertainty in economic predictions.
- Easily accessible data allowing fast assessment of feasible compressor types and better cost correlations considering compression ratio and volumetric flowrate would be of great help to practitioners.
- There is little industrial experience with working fluids for use temperatures of 110°C and higher. While new working fluids like the HFO R1233zd(E) are promising, their high price poses a hurdle for large-scale application.
- The economic results presented here are very sensitive to the absolute level of energy prices as well as the ratio of steam to electricity cost. Rising energy prices and higher relative steam cost favor VR or HP designs.

The data in **Fig. 5** were computed without considering any additional CO_2 surcharge. It is to be expected, that the efforts to reduce worldwide greenhouse gas emissions will lead to additional cost for CO_2 emissions. Any CO_2 surcharge will lead to higher energy cost and therefore improve the economics of VR and HP configurations. Due to higher temperature lift, the HP configurations need larger compressor power (see **Fig. 4a**) and consequently cause higher CO_2 emissions. CO_2 pricing may therefore shift the economic ranking in favor of the VR configurations. If green electric power is supplied, however, CO_2-neutral separation with zero additional CO_2-cost is enabled for VR as well as HP configurations.

Conclusion

Simulation results for vapor recompression and heat pump configurations in a vacuum distillation have been reported. It has been shown that both options significantly reduce the CO_2-footprint and may even become CO_2-neutral, if sustainable green electric power is supplied.

If the allowable operating range is explored, economic VR designs are possible, although the total investment for the separation step is considerably increased. A comprehensive evaluation of the merits of VR and HP options requires preliminary investment and energy cost estimates. This assessment needs to be performed in early design phases, since the impact on plant layout, equipment design and cost is considerable.

In most separations, the practical application of VR and HP technology will be more difficult than in the example presented here. In face of rising energy cost and the trend to electrification of separation processes, economic designs may be developed even in challenging separations. In wide boiling systems, a VR scheme feeding an intermediate side-reboiler in the stripping section is promising while a multi-stage compressor may be designed to feed vapor at different temperature levels to side and bottom reboilers. If a large temperature difference is caused by a limited amount of low-boiler in the feed, a vapor side-stream may be taken out of the rectifying section and compressed to heat the reboiler, while the low-/middle boiler separation is carried out in a column section on top of the heat-pumped column.

The main finding of this paper is that CO_2-saving and energy-conserving VR and HP systems are not limited to high pressure systems and may be successfully applied to vacuum systems. Heat pump configurations may show better economics than vapor recompression. This is contrary to first intuition since additional equipment is required. This finding emphasizes the importance of selecting an optimum working fluid for the task at hand. Cost of new working fluids like HFOs may be substantial and must be weighed against their thermodynamic properties.

Abbreviations

EB	Ethylbenzene
GWP	Global Warming Potential
HIDIC	Internally Heat-Integrated Column
HP	Heat Pump
ODP	Ozone Depletion Potential
POT	Pay Out Time
NPV	Net Present Value
SM	Styrene monomer
VR	Vapor Recompression

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